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Computational technique – A promising pathway for drug discovery: A case study

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Drug discovery is a complex process which involves an interdisciplinary approach to design effective feasible drugs (1). The development of new drugs with potential therapeutic applications is one of the most complex process in the pharmaceutical industry (2). Millions of dollars and man hours are dedicated to the discovery of new therapeutic agents. Rational drug discovery process combat and supersede the conventional process with the advent of proteomic, genomic and structural information (3).

The computational techniques and informatics assist in predicting the 3D structures, the active site, the binding modes of molecules and the ADME properties. The paramount of work is evident from recent publications in this area (4, 5 and the references therein). The present work showcases the application of structure based drug designing techniques, in the identification of new molecular entities with potential therapeutic value with reference to cancer and tuberculosis.

Novel proteins in Mycobacterium tuberculosis are targeted, their 3D structure evaluated, active site identified, virtual screening carried out using Glide software to identify novel leads to inhibit the target proteins. A similar procedure was also applied to the proteins which play an important role in apoptotic pathway. The identified lead molecules were synthesized and their biological activity tested which show promising results. These new molecular entities offer promising therapeutics for further stage of drug discovery.

Sodium alginate based new bioadhesive and rapid oromucosal absorptive sublingual tablet system for intraoral drug delivery

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Oromucosal delivery of drugs promotes rapid absorption and high bioavailability, with subsequent almost immediate onset of pharmacological effect. However, many oromucosal delivery systems are compromised by the possibility of the patient swallowing the active substance before it has been released and absorbed locally into the systemic circulation. With this approach, optimal exposure of active substances to the dissolving fluids is combined with Bioadhesive retention of drug in the oral cavity. This paper introduces a new tablet system for sublingual administration and rapid drug absorption. The tablet is based on an ordered interactive mixture of components, consisting of carrier particles partially covered by fine dry particles of the drug, in this case piroxicam. In the interests of increasing retention of the drug at the site of absorption in the oral cavity, a Bioadhesive component was also added to the carrier particles. Tablets containing 5, 10, 15 and 20 mg of piroxicam were tested in vitro. The tablets disintegrated rapidly and dissolution tests revealed that piroxicam was dissolved from the formulation almost instantly. These results indicated that the bioadhesive component prevented the piroxicam from being swallowed (the fraction swallowed was considered smaller compared to other mucosal delivery systems), without hindering its release and absorption. This new sublingual tablet formulation may also hold potential for other substances where a rapid onset of effect is desirable.